Recent Developments in the Characterization and Applicationof Ultrananocrystalline Diamond Films*

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Phase-pure ultrananocrystalline diamond (UNCD) films are remarkable materials whose synthesis has been made possible by a new CVD process that uses carbon dimer, C_2, as a growth and nucleation species. The elucidation of the growth mechanism that underlies this process has required detailed tight-binding density functional molecular dynamics calculations (M. Sternberg, et al.). These allow one to glimpse the incipient formation of (4,4) nanotube segments, which rebond to the diamond lattice as additional C_2 inserts into the carbon-carbon bonds of the (110) surface to form a completed monolayer. Similar calculations (P. Zapol, et al.) carried out on UNCD allow precise determination of the energies of the electronic states introduced into the band gap of diamond by virtue of the fact that carbon at the grain boundaries is largely three rather than four coordinated. Additional calculations show that nitrogen can be incorporated into the grain boundaries with 3-5 ev less energy expenditure than is required for substitution into bulk diamond leading to the formation of electronic states that appear to adopt doping configurations. Studies by TEM techniques (J. P. Birrell, J. M. Gibson, et al.) of UNCD microstructural charges accompanying nitrogen addition have been observed and will be discussed. These theoretical and experimental insights help one to understand the remarkable four-to-five order of magnitude increases in electrical conductivity observed on adding nitrogen to the UNCD synthesis gas. Hall measurements confirm that n-type doping of diamond has been achieved.

The enhancement of fracture toughness due to π-bonded carbon at the grain boundary combines synergistically with UNCD's surface smoothness and hardness, which approaches that of single-crystal diamond, to result in a material with superior mechanical properties. The chemical inertness and high overpotential for the evolution both of hydrogen and oxygen suggests that UNCD makes excellent coatings for corrosion protection, as well as functioning as a superior electrochemical electrode. The ability to coat complex shapes conformally together with fabricability via photolithography and selective etching makes UNCD a highly suitable new MEMS material for demanding device applications. The many unique properties of UNCD films provide ample opportunities for the exploration of diverse fields of use. Exemplars of applications of UNCD films in the areas of electrochemistry, electron emission, tribology, and MEMS will be discussed.

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